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SOME COMPARISON THEOREMS ON MOMENTS IN THE GROUND STATE AND FIRST RADIAL EXCITED STATES OF A TWO-BODY SYSTEM

A. Martin
CERN - Geneva

ABSTRACT

We prove and extend some conjectures by Dib, Franzini and Gilman on the comparison of expectation values of r^{ν} in the ground state and the first radial excited state of a two-body system for a given, non-zero angular momentum. One of the by-products is that for usual potentials, the overall splitting of the P states is likely to be smaller for the excited state than for the ground state.

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Recently, Dib, Gilman and Franzini [1] have studied the P state splittings by spin-dependent interactions in quarkonium, both for the ground state and for the first radial excited state. On this occasion, they have made interesting numerical observations on the ratios

$$R(\nu) = \frac{\langle r^{\nu} \rangle_{\text{first radial excited state}}}{\langle r^{\nu} \rangle_{\text{ground state}}} \tag{1}$$

in particular for $\nu = -1$ and $\nu = -3$. Here we would like to prove these conjectures, made essentially for power potentials, and try also to generalize to larger classes of potentials.

The starting point is a sum rule which is based on the well-known formula for the wave function at the origin for the $\ell = 0$ partial wave (we take $2\mu = \hbar = 1$)

$$|u'(0)|^2 = \int u^2 \frac{dV}{dr}\, dr \tag{2}$$

If we consider now a state with angular momentum $\ell > 0$ (strictly!) we can think of it as an $\ell = 0$ state with an effective potential

$$W(r) = V(r) + \frac{\ell(\ell+1)}{r^2} \tag{3}$$

where V is a "good" potential, such that $\lim_{r\to 0} r^2 V = 0$, and then, since the reduced wave function behaves as $r^{\ell+1}$, $u'(0) = 0$. Hence we get

$$0 = \int u^2 \left[\frac{dV}{dr} - 2\,\frac{\ell(\ell+1)}{r^3} \right] dr \tag{4}$$

This sum rule can be found in a physics report by Grosse and myself [2] and has also recently been rederived independently by Cahn [3].

From the sum rule, one obtains in particular two simple results:

i) for the logarithmic potential, $V = \lambda \log r$ we get, for <u>any</u> state

$$\lambda \left\langle \frac{1}{r} \right\rangle = 2\,\ell(\ell+1) \left\langle \frac{1}{r^3} \right\rangle \tag{5}$$

and therefore

$$R(-1) = R(-3) \quad , \tag{6}$$

or, for a given ℓ,

$$\frac{\left\langle \frac{1}{r} \right\rangle}{\left\langle \frac{1}{r^3} \right\rangle} = \text{const.},$$

independent of the radial excitation.

ii) For the linear potential, $V = \mu r$

$$R(-3) = R(0) = 1 \quad , \tag{7}$$

since the wave function is normalized. So $\langle 1/r^3 \rangle$ is independent of the radial excitation.

We would like to go beyond these simple observations made also independently by R. Cahn [3]. The strategy we shall use follows essentially the techniques developed in Ref. [2]. First we notice that $R(\nu)$ cannot take three times the same value, i.e., $R = R(\nu_1) = R(\nu_2) = R(\nu_3)$, with $\nu_1 > \nu_2 > \nu_3$, is impossible. Then we would have

$$\int (u_1^2 - R u_0^2) \left[r^{\nu_1} + A r^{\nu_2} + B r^{\nu_3} \right] dr = 0, \tag{8}$$

where u_0 is the ground state wave function and u_1 is the first radial excitation. $u_1^2 - R u_0^2$ vanishes at most twice for $0 < r < \infty$. By combining the Schrödinger equations

$$-u_1'' + \left(V(r) + \frac{\ell(\ell+1)}{r^2} \right) u_1 = E_1 u_1$$

$$-u_0'' + \left(V(r) + \frac{\ell(\ell+1)}{r^2} \right) u_0 = E_0 u_0$$

we get

$$-u_0 u_1' + u_1 u_0' = (E_1 - E_0) \int_0^r u_1 u_0 \, dr' = -(E_1 - E_0) \int_r^\infty u_1 u_0 \, dr'$$

hence, if r_0 is the unique zero of u_1,

$\left|\frac{u_1}{u_0}\right|$ decreases for $r < r_0$

$\left|\frac{u_1}{u_0}\right|$ increases for $r > r_0$

If we restrict ourselves to potentials such that $V(r)$ increases to $+\infty$ and $V(r)/r^2 <$ const., $|u_1/u_0|$ increases from zero to infinity in the interval $r_0 < r < \infty$. Indeed, it can be shown [2] then that the WKB approximation is valid for $r \to \infty$ and hence

$$\left|\frac{u_1}{u_0}\right| \sim \text{const} \exp\left[\int_c^r \frac{E_1 - E_0}{2\sqrt{V(r')}}\, dr'\right] \tag{9}$$

The integral under the exponent diverges if $V(r)/r^2$ remains bounded. Therefore, $u_1^2 - Ru_0^2$ has one and only one zero in $r_0 < r < \infty$.

The same result holds if $V(r) \to 0$, because then

$$\left|\frac{u_1}{u_0}\right| \sim \text{const} \exp\left[r\left(\sqrt{-E_0} - \sqrt{-E_1}\right) + \frac{1}{2}\int^r V(r')\,dr'\left[\frac{1}{\sqrt{-E_0}} - \frac{1}{\sqrt{-E_1}}\right]\right]. \tag{10}$$

Now the quantity $$r^{\nu_1} + A r^{\nu_2} + B r^{\nu_3}$$

vanishes at most <u>twice</u> in $0 < r < \infty$. If $u_1^2 - Ru_0^2$ vanishes only once, at $r = r_1$ we can take $B = 0$ and adjust A so that $r_1^{\nu_1} + Ar_1^{\nu_2} = 0$. Then

$$\int \left(u_1^2 - R u_0^2\right)\left(r^{\nu_1} + A r^{\nu_2}\right) dr$$

is <u>positive</u> and therefore

$$R(\nu_1) \neq R(\nu_2)$$

If $u_1 - Ru_0^2$ vanishes twice, at $r = r_1$ and $r = r_2$, we can solve for A and B so that

$$r_1^{\nu_1}+A r_1^{\nu_2}+B r_1^{\nu_3} = r_2^{\nu_1}+A r_2^{\nu_2}+B r_2^{\nu_3} = 0 .$$

Then we find that the integral (8) is positive. Therefore it is impossible to have

$$R(\nu_1) = R(\nu_2) = R(\nu_3) .$$

Assuming $V(r)/r^2$ bounded for $r \to \infty$, $|u_1/u_0|$ goes to infinity for $r \to \infty$ and it follows from this that $R(\nu) \to +\infty$ for $\nu \to \infty$. Indeed given M arbitrary, we can find R so that $|u_1/u_0|^2 > M$ for $r > R$. Then

$$R(\nu) > \frac{M \int_R^\infty u_0^2 \left(\frac{r}{R}\right)^\nu dr}{\int_0^R u_0^2 \left(\frac{r}{R}\right)^\nu dr + \int_R^\infty u_0^2 \left(\frac{r}{R}\right)^\nu dr} .$$

For $\nu \to \infty$

$$\int_0^R u_0^2 \left(\frac{r}{R}\right)^\nu dr \to 0$$

and

$$\int_R^\infty u_0^2 \left(\frac{r}{R}\right)^\nu dr \to \infty .$$

Hence, given ε, $R(\nu) > M-\varepsilon$ for ν big enough. Since M is as large as we wish we deduce that $R(\nu) \to +\infty$. $R(\nu)$ is defined for $\nu \geqslant -(2\ell+3)$ because of the behaviour of u_0 and u_1 at the origin.

From the previous results we deduce that there are only two possibilities

- Either $R(\nu)$ is monotonously increasing from $\nu = -(2\ell+3)$ to $\nu = \infty$
- or $R(\nu)$ has a unique minimum. This means that we have always

$$R(\nu_2) < \sup \{ R(\nu_1) , R(\nu_3) \} , \qquad (10)$$

if $\nu_1 > \nu_2 > \nu_3$.

If we take the moments considered by Dib, Franzini and Gilman, we have for instance:

$$\frac{\left\langle \frac{1}{r} \right\rangle_1}{\left\langle \frac{1}{r} \right\rangle_0} < \sup \left\{ 1, \frac{\left\langle \frac{1}{r^3} \right\rangle_1}{\left\langle \frac{1}{r^3} \right\rangle_0} \right\} \tag{11}$$

Similarly one has

$$R(-1) < \sup \{ 1, R(-2) \} \tag{12}$$

This is amusing for

$$R(-2) = \frac{(2\ell+1) \int \frac{u_1^2 dr}{r^2}}{(2\ell+1) \int \frac{u_0^2 dr}{r^2}} = \frac{\frac{dE_1}{d\ell}}{\frac{dE_0}{d\ell}} \tag{13}$$

If we look at the upsilon spectrum we have

$$\frac{E(l=1, n=1) - E(l=0, n=1)}{E(\ell=1, n=0) - E(\ell=0, n=0)} \cong \frac{220 \text{ MeV}}{440 \text{ MeV}} = 0.5 . \tag{14}$$

So it is extremely likely that R(-2) is less than unity and we conclude that for the upsilon P states it is very probable that

$$\frac{\left\langle \frac{1}{r} \right\rangle_{n=1}}{\left\langle \frac{1}{r} \right\rangle_{n=0}} < 1 . \tag{15}$$

Remarkably, we reach this conclusion without knowing the potential.

Now we shall make use of the sum rule (4) and first consider for simplicity attractive power potentials

$$V = \varepsilon(\alpha)\, r^{\alpha} \quad , \tag{16}$$

where ε is the sign function. Then we get

$$\alpha\, \varepsilon(\alpha) \langle r^{\alpha-1} \rangle = 2\, \ell(\ell+1) \langle r^{-3} \rangle . \tag{17}$$

Hence

$$R(\alpha-1) = R(-3) .$$

Then, from property (10), we get by choosing conveniently ν_1, ν_2, ν_3

$$R(\nu) \leqslant 1 \quad \text{for } -3 \leqslant \nu \leqslant 0 \quad \text{if } \alpha \leqslant 1 \quad , \tag{18}$$

$$R(-3) > 1 \quad \text{if } \alpha > 1 \quad , \tag{19}$$

$$R(-1) > R(-3) \quad \text{if } \alpha < 0 \quad , \tag{20}$$

$$R(-1) < R(-3) \quad \text{if } \alpha > 0 \quad . \tag{21}$$

Can we say something for non power potentials? Here we shall follow what has been done in the special case of R(-2) in Ref. [2] p. 355.

First we compare R(-3) to 1. Let us prove that if $(d/dr)r^4(d^2V/dr^2)$ has a given sign for all r, R(-3) differs from unity. Assume R(-3) = 1 then

$$0 = \int \left(u_1^2 - u_0^2\right) \left[\frac{dV}{dr} + \frac{A}{r^3} + B \right] = 0 \tag{22}$$

We can adjust A and B so that $dV/dr + A/r^3 + B$ vanishes at $r = r_1$ and r_2, the zeros of $u_1^2 - u_0^2$ (if there is only one zero we can take A = 0). Then

$$\frac{d}{dr}\left[\frac{dV}{dr} + \frac{A}{r^3} + B \right] = \frac{d^2V}{dr^2} - \frac{3A}{r^4} = \frac{z}{r^4}$$

and

$$z' = \frac{d}{dr} r^4 \frac{d^2V}{dr^2} = r^4 V''' + 4r^3 V'' .$$

If z' has a constant sign, z is monotonous and $dV/dr + A/r^3 + B$ vanishes at most twice. Therefore, it vanishes only at $r = r_1$ and $r = r_2$ and the integral has a constant sign, which contracts (22). To find the sign of R(-3)-1 we use the family of potentials

$$V_\lambda = \lambda r^\alpha + (1-\lambda)\, V(r) \;.$$

R(-3) is a continuous function of λ and for $\lambda = 0$ the sign of R(-3) is known. Choosing conveniently α we get

$$R(-3) > 1 \qquad \text{if} \quad rV''' + 4V'' > 0 \tag{23}$$

$$R(\nu) < 1 \quad \text{for} \; -3 \leqslant \nu < 0 \quad \text{if} \quad rV''' + 4V'' < 0 . \tag{24}$$

(In particular R(-3) < 1, R(-1) < 1.) If it happens that $u_1^2 - u_0^2$ has a single zero (which could be the case if V" < 0) then it suffices to take V" < 0 to get (24), however, V" < 0 follows from $(d/dr)r^4(d^2V/dr^2) < 0$ by integration.

Most existing potential models of quarkonium satisfy condition (24). For instance, this is the case of power superpositions with $\alpha \leqslant 1$. In physical terms the meaning of (24) is that, except for miraculous sign arrangements, we expect the overall P state splittings to shrink when one goes from the ground state to the first radial excitation, since in practically all potential models the quantities controlling the fine splittings are expectation values of r^ν, $-3 < \nu < 0$, or superpositions. The special case $\nu = -2$ in (24) was already treated in Ref. [2]. However, the condition found was slightly different:

$$R(-2) = \frac{\frac{dE_1}{d\ell}}{\frac{dE_0}{d\ell}} < 1 \qquad \text{if} \quad 3V'' + rV''' < 0 .$$

In reality, a subtlety was overlooked: sometimes $u_1^2 - u_0^2$ has only <u>one</u> zero and then one must make sure that the quantity multiplying it has only <u>one</u> zero. By multiplying 3V"+rV" by r^2 and integrating, one gets V" < 0 which is sufficient, <u>provided</u> $\lim_{r\to 0} r^3 V'' = 0$. This is not the case if the potential is singular like 1/r or worse. So condition 4V"+rV''' < 0 is much better, because it suffices for all cases such that $\lim_{r\to 0} r^2 V = 0$. Almost all potentials used for quarkonium satisfy this condition and by integration we get

$$E(n=1, \ell=1) - E(n=1, \ell=0) < E(n=0, \ell=1) - E(n=0, \ell=0)$$

which is true for the upsilon system as seen in (14).

One would be tempted to believe that (24) would hold under the weaker condition $V'' < 0$. This does not seem to be the case. Indeed, from (4) one can get, by integration by parts

$$2\,\ell(\ell+1)\int \frac{u_1^2-u_0^2}{r^3}\,dr = \int_0^\infty V''(r)\, I(r)\, dr \tag{25}$$

where

$$I(r) = \int_r^\infty (u_1^2-u_0^2)\,dr' = -\int_r (u_1^2-u_0^2)\,dr'$$

In the limit case $V(r) = r$, $u_1^2-u_0^2$ vanishes <u>twice</u> for ℓ strictly positive. Otherwise one would get a contradiction with the sum rule (4). Then $I(r)$ is not positive definite and this will also be the case for potentials close to the linear potential like

$$V = r - \varepsilon\,\theta(r-R)\,,$$

for ε sufficiently small. Then one can get an arbitrary sign for (25) by choosing R conveniently.

The other result to generalize to non power potential concerns the comparison of $R(-1)$ and $R(-3)$. Again we assume that $R(-1) = R(-3) = R$ and get

$$\int (u_1^2 - R\,u_0^2)\left[\frac{dV}{dr} + \frac{A}{r^3} + \frac{B}{r}\right] dr = 0$$

We adjust A and B in the bracket so that it vanishes at $r = r_1$ and r_2 the zeros of $u_1^2-Ru_0^2$ and invent a sufficient condition to make sure that it does not vanish anywhere else. Clearly this condition is

$$\frac{d}{dr}\, r^3 \frac{d}{dr}\, r \frac{dV}{dr}$$

of constant sign. Then, using again the trick of the auxiliary power potential we get

$$\begin{aligned} R(-1) &> R(-3) \quad \text{if} \quad \frac{d}{dr}\, r^3 \frac{d}{dr}\, r \frac{dV}{dr} < 0 \\ R(-1) &< R(-3) \quad \text{if} \quad \frac{d}{dr}\, r^3 \frac{d}{dr}\, r \frac{dV}{dr} > 0\,. \end{aligned} \tag{26}$$

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